Relationships among coefficients in deterministic and stochastic transient diffusion

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Systems are studied in which transport is possible due to large extension with open boundaries in certain directions but the particles responsible for transport can disappear from it by leaving it in other directions, by chemical reaction or by adsorption. The connection of the total escape rate, the rate of the disappearance and the diffusion constant is investigated. It leads to the observation that the diffusion coefficient defined by $\langle x^2 \rangle$ is in general different from the one present in the effective Fokker-Planck equation. The result makes it possible to generalize the Gaspard-Nicolis formula for deterministic systems to this transient case.

Randomness and diffusion are common features of extended stochastic and chaotic systems [1,2,3,4,5,6,7,8,9]. Among deterministic systems diffusion has been much studied in the Lorentz gas [3,4]. As more simple models proper 1D maps [5,6,7,8] and a 2D map [9] has been introduced, which were built as chains of maps. Ref. [10] has shown a relationship between the diffusion coefficient and microscopic quantities, namely the Liapunov exponent and the Kolmogorov-Sinai entropy referring to the repeller. This was later generalized to other transport coefficients [11] and case of small external field [12]. The Liapunov exponent was independently calculated for the random Lorentz gas [13].

There are systems in which particles can escape in directions transversal to the extension of the system raising interestic problems [14] in the field of transient chaos [15] in particular in the critical case [16,17]. A simple example is a channel in a mesoscopic system modeled by a strip of Lorentz gas with open side boundaries. Another example is the Troll-Smilansky model for chaotic scattering consisting of a 1D infinite periodic array of soft potential valleys, which is a system related to a model of ionization [18,19]. Further example is the motion in an infinite set of resonances in the phase space of Hamiltonian systems when one considers the particle to escape when it leaves the set of chosen resonances [20]. Diffusion has also been investigated on a chaotic saddle in a model for the interaction of a particle with electrostatic wavepacket [21]. Particles can also be lost from the point of view of diffusion by absorption, chemical reaction [22] or by other ways. Particles in such transiently chaotic or stochastic systems can diffuse in the extended direction or directions for some time and then escape either through the ends in the extended direction (if the system is finite) or in the other directions or other ways. Therefore the average period for which they take part in transport is finite, and remains finite even in the limit when the size of the system in the extended direction goes to infinity.

The aim of the present paper is to generalize the Gaspard-Nicolis formula [10] to the case of the above described transient diffusion in deterministic systems. For this purpose it is studied how the total escape rate separates to terms related to the extended and the transversal direction. This investigation is made in a general way leading to interesting results for both deterministic and stochastic systems. For simplicity the system is assumed to possess one extended direction with a discrete translational symmetry, and in most of the considerations here, an inversion symmetry that reverses the extended direction. For sake of convenience the primitive cells with respect to the translational symmetry shall be labeled by a discrete variable x that is monotonous in the extended direction. The rest of variables specifying the state of the particle shall be assembled in y. It is convenient to show the choice of x and y in case of the strip of Lorentz gas. Here, as in general, it is easier to study the system in discrete instead of continuous time. Taking the surfaces of the disks as Poincaré surface the state of the particle on it can be given by the coordinates x, q, α and β. By x we mean the ordered label of the periods of the structure. q is a label of the disk inside one period, α is the angle of position on the disk and β is the angle of reflection. Then y corresponds to (q, α, β).

The general evolution equation for the probability density $\phi_t(x, y)$ of the particle can be written as

$$\phi_{t+1}(x,y) = \sum_{j=-J}^{J} \sum_{y'} w_{j,y,y'} \phi_t(x-j, y') \ , \qquad (1)$$

where, if y contains continuous variables one can consider the sums as integrals over the continuous components or one can use coarse graining with arbitrary precision. Here $\phi_t = 0$ if the argument falls outside the region of the system. The maximal jump J can be assumed to be finite, or the transition probability $w_{j,y,y'}$ to decay fast in j. The translational symmetry is implied in the form of (1), while an inversion symmetry can be written as $w_{j,y,y'} = w_{-j,Ty,Ty'}$, where $T^2 y = y$ for every y.

Two representative classes of such systems can one keep in mind here. The first is a 2D random walk in a strip, for simplicity assuming no memory, for which

$$\phi_{t+1}(x,y) = \sum_{j=-J}^{J}\sum_{k=-K}^{K} W_{jk}\phi_t(x-j,y-k) \qquad (2)$$

applies. This can be considered as a rough description of the Lorentz gas strip. The inversion symmetry can be a point inversion or a line inversion symmetry. To give an account of correlation between transitions 1D walks with memory are taken as a second group of examples. Then (1) can be used conceiving y as the memory containing, say, n number of past steps $j_1, j_2, \dots j_n$ and $w_{j_{n+1},y,y'} = P(j_{n+1}|j_n, j_{n-1}, \dots j_1)$ is the conditional probability of the next step. The inversion symmetry implies $P(j_{n+1}|j_n, j_{n-1}, \dots j_1) = P(-j_{n+1}|-j_n, -j_{n-1}, \dots -j_1)$.

For general considerations we shall return to (1) taken without restriction to 1D. For the diffusion process the long time behavior of the system is important. That is governed by the leading eigenfunction of the right hand side of (1), i. e. the solution ϕ_t for which $\phi_{t+1} = e^{-\kappa}\phi_t$ and the total escape rate κ is minimal. This ϕ_t shall be called the asymptotic state. The boundary of the system should also show the symmetry, so the region of the system should be defined by independent conditions in x and y ($x \in R_x$ and $y \in R_y$). If the particle from a point (x_0, y_0) jumps to a point (x, y), for which $y \notin R_y$ the particle shall be considered to escape in y direction, while in case $y \in R_y$ but $x \notin R_x$ it escapes in x direction.

To find the relation of the escape rates and the diffusion coefficient is simple in certain cases but is problematic in general. It is enlightening to study the simple cases first. These are the ones in which the asymptotic solution separates as a product $\phi(x,y) = \psi(x)\omega(y)$. This happens if the transition probability matrix is a sum of diadic products $w_{jyy'} = \sum_s u_j^{(s)} v_{yy'}^{(s)}$ and the partial diffusion equations in x direction have a common leading eigenfunction, i. e. $\sum_j u_j^{(s)}\psi(x-j) = \mu_s\psi(x)$ such that for every s μ_s is the maximal eigenvalue. This property shall be denoted by S_x. It is easy to see that in this case the eigenvalue equation in y direction $\sum_{y's} v_{yy'}^{(s)}\mu_s\omega(y') = e^{-\kappa}\omega(y)$ determines ω and $e^{-\kappa}$. An example for this case among the 2D walks (2) is a walk on a square lattice $[1, L] \otimes [1, M]$ with

$$\{W_{jk}\}_{-1,-1}^{1,1} = \begin{pmatrix} 0 & q & 0 \\ 0 & r & 0 \\ p & 0 & p \end{pmatrix} = \begin{pmatrix} q \\ r \\ 0 \end{pmatrix} \circ (010) + \begin{pmatrix} 0 \\ 0 \\ p \end{pmatrix} \circ (101) \qquad (3)$$

whose solution reads
$\phi = \sin\left(\pi\frac{x}{L+1}\right)\left[2\frac{p}{q}cos\left(\frac{\pi}{L+1}\right)\right]^{y/2}\sin\left(\pi\frac{y}{M+1}\right)$.

Another possibility is when the eigenmode is common in y direction, i. e. $\sum_{y'} v_{yy'}^{(s)}\omega(y') = \nu_s\omega(y)$ (property S_y). Then $\sum_{js} u_j^{(s)}\nu_s\psi(x-j) = e^{-\kappa}\psi(x)$ determines ψ and $e^{-\kappa}$. When the properties S_x and S_y are both satisfied then $e^{-\kappa} = \sum_s \mu_s\nu_s$.

To obtain an evolution equation of the distribution on large scale in x direction in either of the above cases with $\phi(x,y) = \psi(x)\omega(y)$ one has to study the evolution of ψ. It is convenient to choose the normalization $\sum_y \omega(y) = 1$, since then $\psi(x) = \sum_y \phi(x,y)$. Using this equation and (1) one obtains

$$\psi_{t+1}(x) = \sum_j \tilde{w}_j\psi_t(x-j)\ , \quad \tilde{w}_j \equiv \sum_{yy'} w_{j,y,y'}\omega(y')\ . \quad (4)$$

Obviously the probability that a particle at $x_0 = x - j$ does not escape in y direction in the next step is $e^{-\kappa_y} = \sum_j \tilde{w}_j \equiv \sum_{jyy'} w_{jyy'}\omega(y')$, which is independent of x_0. One can separate this escape with substitution $\psi_t(x) = e^{-\kappa_y t}g_t(x)$, which yields $g_{t+1}(x) = \sum_j \tilde{w}_j e^{\kappa_y} g_t(x-j)$. Since this equation describes a random walk and the system is extended in x direction an effective Fokker-Planck equation $g_{t+1}(x) = g_t(x) + D_{FP}g_t''(x)$ is valid on large scales. Returning to ψ it takes the form

$$\psi_{t+1}(x) = \left(1 + D_{FP}\frac{d^2}{dx^2}\right)e^{-\kappa_y}\psi_t(x)\ . \qquad (5)$$

Its dominant solution in case of a channel of length L is

$$\psi_t(x) = e^{-\kappa t}\sin\left(\pi\frac{x}{L}\right)\ , \quad \kappa = \kappa_x + \kappa_y\ , \qquad (6)$$

and $\kappa_x = (\pi^2/L^2)D_{FP} + \mathcal{O}(L^{-3})$, if κ_x is defined such, that $e^{-\kappa_x}$ is the conditional probability that a point does not escape in x direction if it does not escape in y direction. Note, that κ_y may also depend on L.

The general case, when $\phi(x,y) \neq \psi(x)\omega(y)$ is more complicated. The main point is, that κ_y becomes dependent on x and L, the length of the system in x direction. However, in case when L is much larger than the size in other directions and there is an inversion symmetry it shall be shown, that apart from a vicinity of the ends of the channel the deviation of κ_y from a value $\kappa_y^{(\infty)}$ is proportional to $f''(x)/f(x)$. Here $f(x)$ is introduced analogously to $\psi(x)$ as $f(x) = \sum_y \phi(x,y)$ and $\kappa_y^{(\infty)}$ is the value of κ_y for the homogeneous solution in case $L = \infty$. This makes it possible to write down a proper effective Fokker-Planck equation. It is suitable to choose a segment of the system separated by $x = $ const planes, such that its size is still much larger than the transversal size, but much smaller than L. Such a segment feels values $f(x_1)$, $f(x_2)$ of f at its ends with a common exponential decay $e^{-\kappa t}$. It is assumed that the diffusion in the system mixes the contribution of sites with different y coordinates. So systems are excluded in which the particles from one site can not fill the whole system, thereby different initial distributions can lead to different asymptotic states. With this assumption the effect of the transversal distribution $\phi(x,y)/f(x)$ decays fast from the ends of the segment towards its inside. On the other side, in the asymptotic state the transversal distribution at the ends of the segment is almost identical to the one in the middle. Therefore one can expect the distribution in the inside of the segment is determined by the values $f(x_1)$, $f(x_2)$ and the decay rate κ.

Thereby the distribution can have three free parameters. Since the evolution equation (1) is linear in the distribution, the asymptotic distributions ϕ and f can be assumed to have linear combination form

$$\phi(x,y) = [\phi^{(\infty)}(x-x_0,y) + c_1\phi^{(1)}(x-x_0,y) + c_2\phi^{(2)}(x-x_0,y)]e^{-\kappa t} , \quad (7)$$

$$f(x) = [1 + c_1 f^{(1)}(x-x_0) + c_2 f^{(2)}(x-x_0)]e^{-\kappa t} , \quad (8)$$

where $f^{(k)}(x) = \sum_y \phi^{(k)}(x,y)$ for $k = 1,2$ and x_0 is the center of the segment. Here $\phi^{(\infty)}(x,y) = \omega^{(\infty)}(y)$ is the solution in the limit $L \to \infty$ that is independent of x. The corresponding escape rate shall be denoted by $\kappa_y^{(\infty)}$. $\phi^{(1)}$ is the asymptotic solution of (1) with antisymmetric boundary conditions $f(x_1) = -f(x_2)$. This term is responsible for current through the middle of the segment. Starting with a $\phi^{(\infty)}$ alone and symmetric boundary conditions $f(x_1) = f(x_2) = ae^{-\kappa t}$ one observes in general that ϕ in the middle decays faster or slower than on the boundary depending on the sign of $\kappa - \kappa^{(\infty)}$. In the asymptotic state this leads to a hump- or vale-shape term $f^{(2)}$ in f, which corresponds to some $\phi^{(2)}$. The partial distributions can be approximated as $f^{(1)}(x-x_0) = x-x_0$ and $f^{(2)}(x-x_0) = (x-x_0)^2 - b$ in a vicinity of the middle of the segment if $\phi^{(k)}$, $k = 1,2$ are properly normalized. This means, that the general solution is

$$\phi(x,y) = f(x_0)\phi^{(\infty)}(x-x_0,y) + f'(x_0)\phi^{(1)}(x-x_0,y) + \frac{f''(x_0)}{2}(\phi^{(2)}(x-x_0,y) + b\phi^{(\infty)}(x-x_0,y)) \quad (9)$$

in a vicinity of the point x_0. The local rate of escape $\kappa_y(x_0)$ in y direction in the middle can be calculated as

$$1 - e^{-\kappa_y(x)} = \frac{E(x_0)}{f(x_0)} , \quad (10)$$

$$E(x_0) = \sum_y \phi(x_0,y) - \sum_{yy'} w_{jyy'}\phi(x_0,y') , \quad (11)$$

where $E(x_0)$ is the flow of escape in y direction at x_0. Then clearly

$$E(x_0) = E_\infty f(x_0) + E_1 f'(x_0) + \frac{(E_2 + bE_\infty)}{2} f''(x_0), \quad (12)$$

where $E_k, k = \infty, 1, 2$ are constants characteristic of $\phi^{(k)}$, respectively. It can be shown that $E_1 = 0$. To see this one can separate Eq. (1) to terms related to transition from inside of the chosen segment and from outside. Conceiving $\phi_t(x,y)$ as a vector $\Phi = \{\Phi_i\}_i$, where any value of the index i corresponds to a point in (x,y) space inside the segment and assuming the asymptotic state (i. e. $\phi_{t+1} = e^{-\kappa}\phi_t$) one obtains $e^{-\kappa}\Phi_i = \sum_j \tilde{w}_{ij}\Phi_j + \chi_i$. Here $\tilde{w}$ describes the transitions inside, χ the transitions from outside, and $\tilde{w}, \chi$ can be constructed using w and values of ϕ outside but near the boundary of the segment. The solution for Φ is $\Phi = \left(e^{-\kappa}I - \tilde{w}\right)^{-1}\chi$, where I is the unit matrix. The boundary conditions are antisymmetric for the symmetry transformation T in the state $\phi^{(1)}$, thereby χ is also antisymmetric. w and $\tilde{w}$ are symmetric for T. Consequently $\Phi^{(1)}$ and the corresponding $\phi^{(1)}$ are antisymmetric. Therefore (11) yields E_1=0. Using (10) and (12) one obtains

$$\kappa_y(x) = \kappa_y^{(\infty)} + \eta\frac{f''(x)}{f(x)} + \mathcal{O}(L^{-3}) \quad (13)$$

with a suitable constant η, since for large L one expects $f'' = \mathcal{O}(L^{-2})$. This is not valid near the ends of the channel where the middle of the segment can not be placed. Then the analog of the effective Fokker-Planck equation (5) becomes of the from

$$f_{t+1}(x) = \left(1 + D_{FP}\frac{d^2}{dx^2}\right)e^{-\kappa_y(x)}f_t(x) , \quad (14)$$

or, with substitution of (13)

$$f_{t+1}(x) = e^{-\kappa_y^{(\infty)}}\left(1 + (D_{FP} - \eta)\frac{d^2}{dx^2}\right)f_t(x) . \quad (15)$$

It is plausible to assume that a distribution corresponding to (9) sets in earlier in time than the asymptotic state in the extended direction. Then (14,15) are also valid for general $f(x)$ distributions still not in the asymptotic state. (15) shall be applied later for such a case, but here the asymptotic solution is important. It is given by

$$f_t(x) = e^{-\kappa t}\cos\left[\sigma\left(\frac{x}{L} - \frac{1}{2}\right)\right] , \quad (16)$$

with $\kappa = \kappa_y^{(\infty)} - \log[1 - (D_{FP} - \eta)\sigma^2/L^2]$, which is valid inside the channel with a deviation at its ends, such that $f_t(x)$ reaches zero at the ends ($x = 0$ and $x = L$), while (16) takes zero value at $\xi = (1 - \pi/\sigma)L/2$. In the limit $L \to \infty$ the value of ξ becomes constant, since the neighborhood of the channel behaves in the same way in this limit. Therefore $\sigma = \pi + \mathcal{O}(L^{-1})$. Using (13) and (16) one can notice, that $\kappa_y(x)$ is constant apart from the vicinity of the ends of the channel. Its value is

$$\kappa_y^{(L)} = \kappa_y^{(\infty)} - \frac{\pi^2}{L^2}\eta + \mathcal{O}(L^{-3}) , \quad (17)$$

where the notation emphasizes its dependence on L. Using this equation and the ones for κ and σ one obtains the relation of the escape rates with the diffusion coefficient

$$\kappa = \frac{\pi^2}{L^2}D_{FP} + \kappa_y^{(L)} + \mathcal{O}(L^{-3}) . \quad (18)$$

Note, that $(\pi^2/L^2)D_{FP}$ does not give κ_x in general, contrary to (6). Following [10] in case of deterministic process the total escape rate can be related to the Liapunov exponents and the Kolmogorov-Sinai entropy of the repeller, namely, $\kappa = \sum_{\lambda_i>0}\lambda_i - h_{KS}$ [23,24]. This yields the generalization of the Gaspard-Nicolis formula [10]

$$\sum_{\lambda_i>0} \lambda_i - h_{KS} = \frac{\pi^2}{L^2} D_{FP} + \kappa_y^{(L)} + \mathcal{O}(L^{-3}) \ . \qquad (19)$$

One more important question is whether D_{FP} defined as the coefficient in (14) is equal to the one defined by the mean square deviation of x as $\int f_t(x)(x-x_0)^2\,dx/\int f_t(x)\,dx \propto 2D_{msd}t$, starting from a state concentrated in a vicinity of x_0. Introducing $g_t(x) = e^{\kappa_y^{(\infty)}t} f_t(x)$ in Eq. (15) one can eliminate the factor containing $\kappa_y^{(\infty)}$. Then the equation becomes an evolution equation of a diffusion process whose diffusion coefficient

$$D_{msd} = D_{FP} - \eta \qquad (20)$$

is clearly equal to the diffusion coefficient defined for $f_t(x)$ by mean square deviation. So we can see D_{FP} and D_{msd} are in general different. Comparing (19) to the Gaspard-Nicolis formula [10] one can notice that $\kappa_y^{(L)}$ has appeared as an additional term, but using (17) and (20) one can get another form of (19) in which D_{msd} and $\kappa_y^{(\infty)}$ are present instead of D_{FP} and $\kappa_y^{(L)}$:

$$\sum_{\lambda_i>0} \lambda_i - h_{KS} = \frac{\pi^2}{L^2} D_{msd} + \kappa_y^{(\infty)} + \mathcal{O}(L^{-3}) \ . \qquad (21)$$

Numerical calculations have been made to test the validity of the statements for $\kappa_y(x)$ and Eqs. (14,20) in two concrete models.

A, The first model is a 2D random walk on a square lattice $[1,L]\otimes[1,M]$ with

$$\{W_{jk}\}_{-1,-1}^{1,1} = \begin{pmatrix} 0 & 0 & p \\ q & r & q \\ p & 0 & 0 \end{pmatrix} \qquad (22)$$

and $p = 0.1$, $q = 0.2$, $r = 0.4$.

B, The second model is a 1D random walk with two step memory such that $P(j_{t+1}|j_t, j_{t-1}) = R_{j_t j_{t-1}} Q_{j_{t+1} j_t}$ and $R_{+1} = 0.45$, $R_{-1} = 0.9$, $Q_{+1} = 4/9$, $Q_{-1} = 5/9$. To ensure symmetry Q and R depend only on the product in their subscript. $Q_{+1} + Q_{-1} = 1$, therefore R describes the probability that the particle does not escape in y direction and Q describes the relative probability of the steps j_{t+1}. A possibility was given to rest for one step with a probability $g = 0.01$ without changing j_t, j_{t-1}.

In model A $\kappa_y(x)$ was found to decay exponentially to $\kappa_y^{(L)}$ coming from each of the ends towards the inside of the region. In model B $\kappa_y(x)$ is constant for $x = 2, 3, \dots L-1$ and has different values only at the endpoints. In both models κ and $\kappa_y(x)$ have been measured. D_{FP} has been calculated from them by (18) for large L and η from the L-dependence of $\kappa_y^{(L)}$ by (17). D_{msd} has been determined independently measuring $\langle (x-x_0)^2\rangle$ for a well concentrated initial distribution. The results satisfy (20) up to the expected precision (5 digits). In case of model A D_{FP} has also been calculated by $i(x) = D_{FP}(f(x) - f(x+1))e^{-\kappa_y(x)}$, where $i(x)$ is the current between sites at x and $x+1$. The results of this match the ones by (18), thereby confirming the validity of (14) and (18), which was used in (19).

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